

TAD04 – (A5 Notes) Nuclear Magnetic Resonance (NMR) Spectroscopy

Name

1. A.5.1 Deduce the structure of a compound given information from its ^1H NMR spectrum. (3) *Students will only be assessed on their ability to deduce the number of different hydrogen (proton) environments and the relative numbers of hydrogen atoms in each environment. They should be familiar both with a word description of a spectrum and with a diagram of a spectrum, including an integration trace. The interpretation of splitting patterns will not be assessed.*

a. Quantum Number Review (NOT an IB topic)

i. Principle Quantum Number

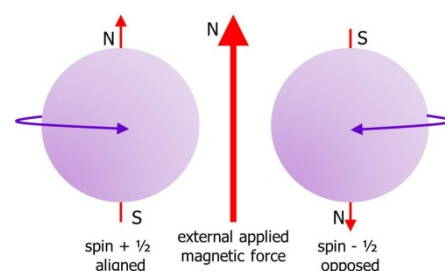
ii. Angular-momentum Quantum Number

iii. Magnetic Quantum Number

iv. Magnetic Spin:

v. How can this be related to NMR?

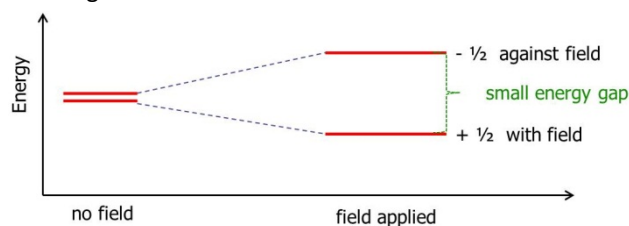
b. Spin of a Proton



i. What must be true of visible nuclei?

ii. Why does the direction of spin dictate the magnetic field produced?

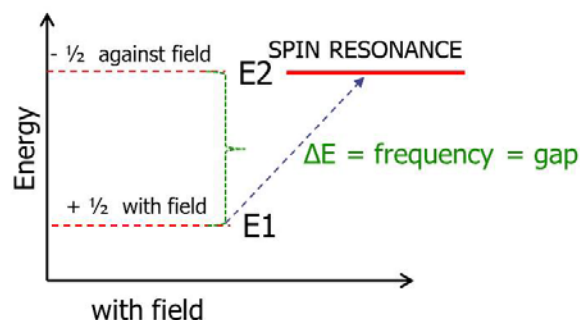
iii. When a magnetic field is applied, protons spin with or against the field.



1. Majority spin with the field

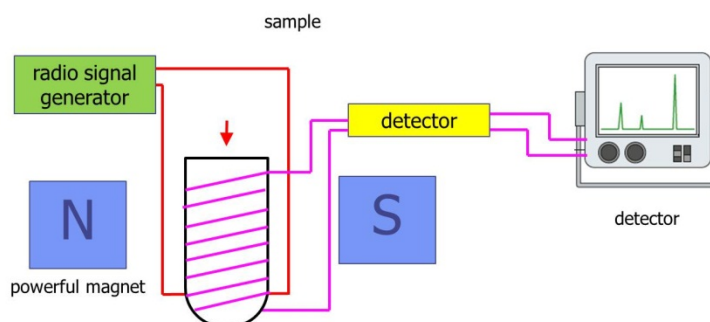
2. Low abundance spin against the field

- iv. Explain how **spin resonance** can be achieved by the addition of a low frequency electromagnetic wave. Discuss the magnitude of this frequency:



- c. Discuss how a sample is prepared and collected for NMR spectroscopy:

- d. Diagram of an NMR Spectrometer:



- e. Give two simple examples of hydrogen protons that will have a different spins for ^1H NMR spectroscopy:

- f. What is the reference point for ^1H NMR?

- g. What is the **chemical shift** and how is it calculated?

- h. Table of ^1H NMR Data Peaks (also Table 18 in IB Data Booklet – 2009)

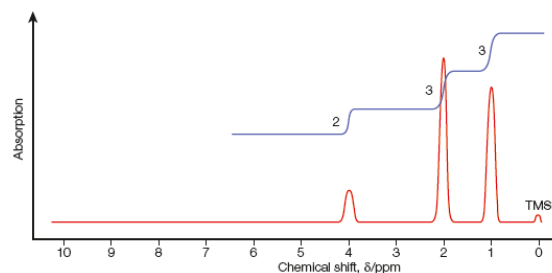
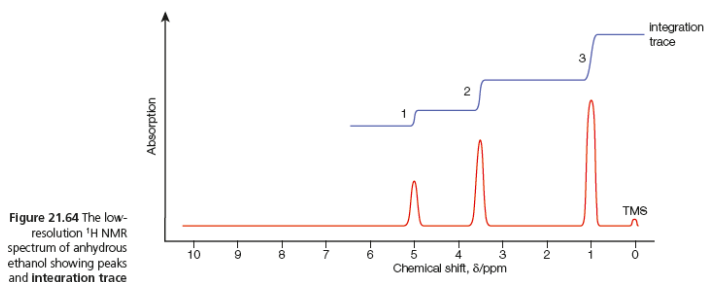
Type of Proton	Shift	Type of Proton	Shift
	0.9-1.0		1.8-3.1
	1.3-1.4		3.5-4.4
	1.4-1.6		3.3-3.7
	2.0-2.5		3.3-4.0
	2.2-2.7		3.8-4.1
	2.5-3.5		9.0-13.0
			4.0-12.0

- i. What is the integration Trace (ratio)?

j. Determine the isomer of each compound:

i. $\text{C}_2\text{H}_6\text{O}$

ii. $\text{C}_4\text{H}_8\text{O}_2$



2. A.5.2 Outline how NMR is used in body scanners. (2) **Aim 8:** Protons in water molecules within human cells can be detected by magnetic resonance imaging (MRI), giving a three-dimensional view of organs in the human body.

a. In general, explain the process of medical Magnetic Resonance Imaging:

b. What can an MRI scan “see”?

c. What are the common uses for an MRI?

d. Setup for Medical MRI:

